LA-UR-13-21209
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Title: Materials @ LANL Overview

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Intended for: Capabilities marketing material for industrial sponsors and collaborations

Materials@LANL

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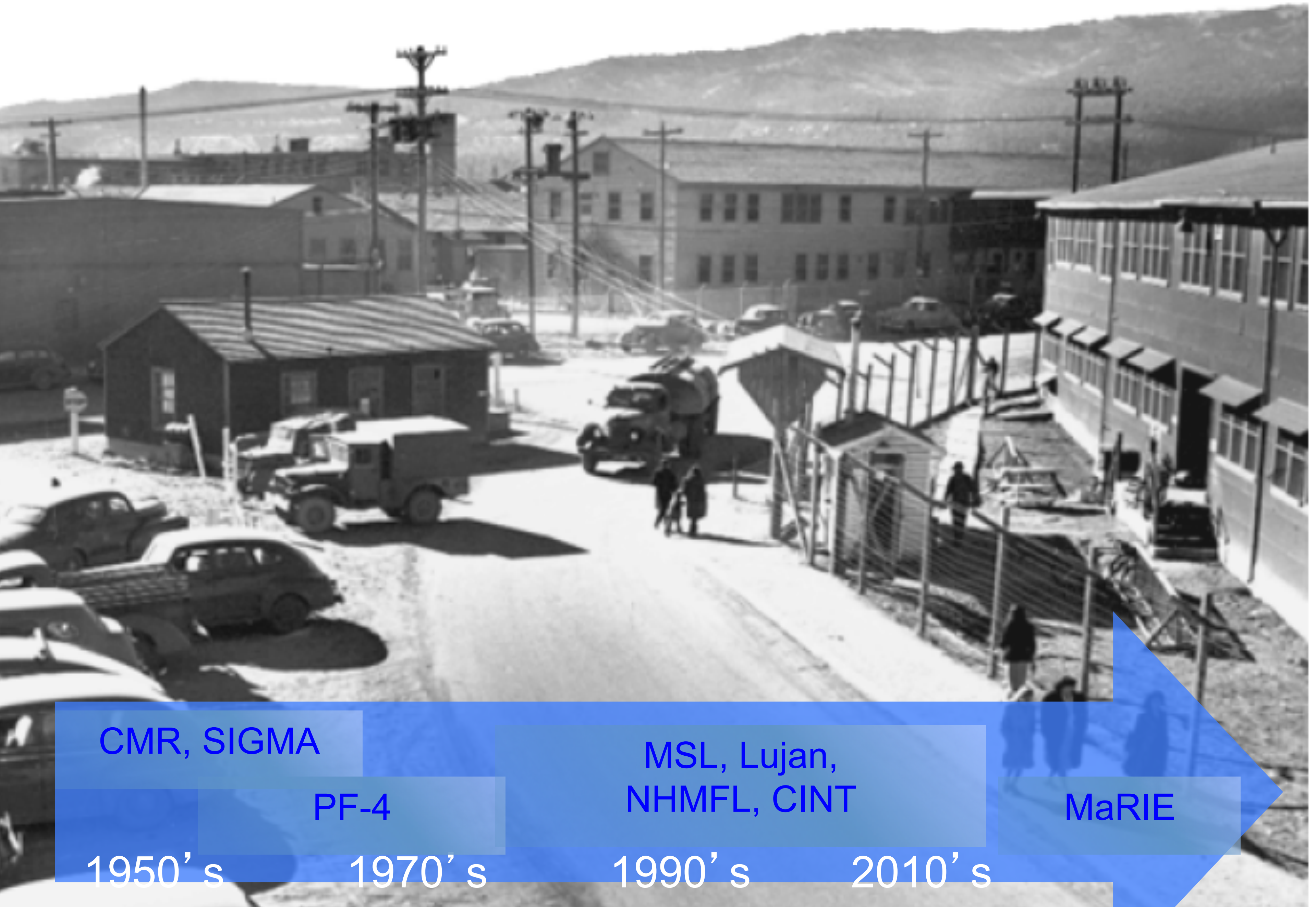
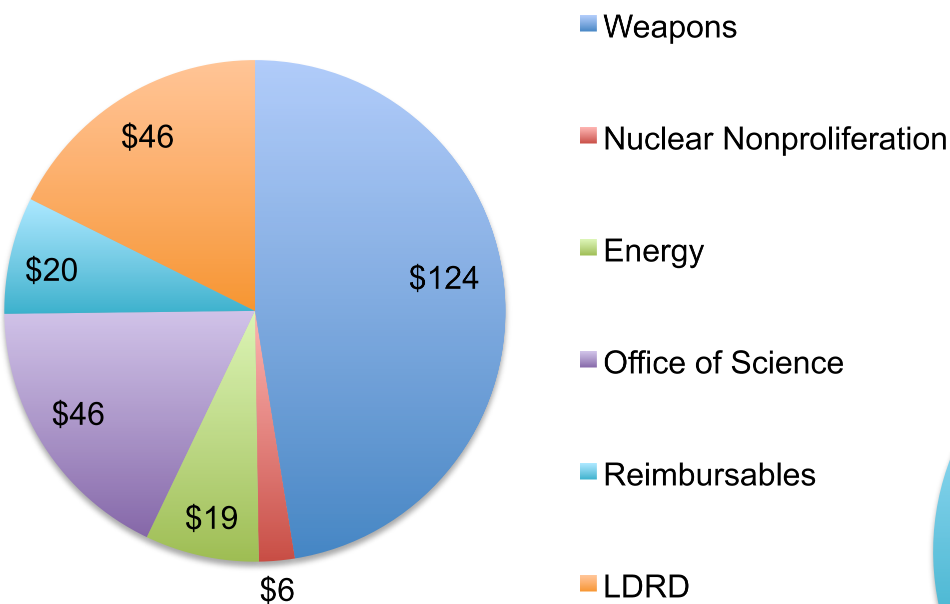
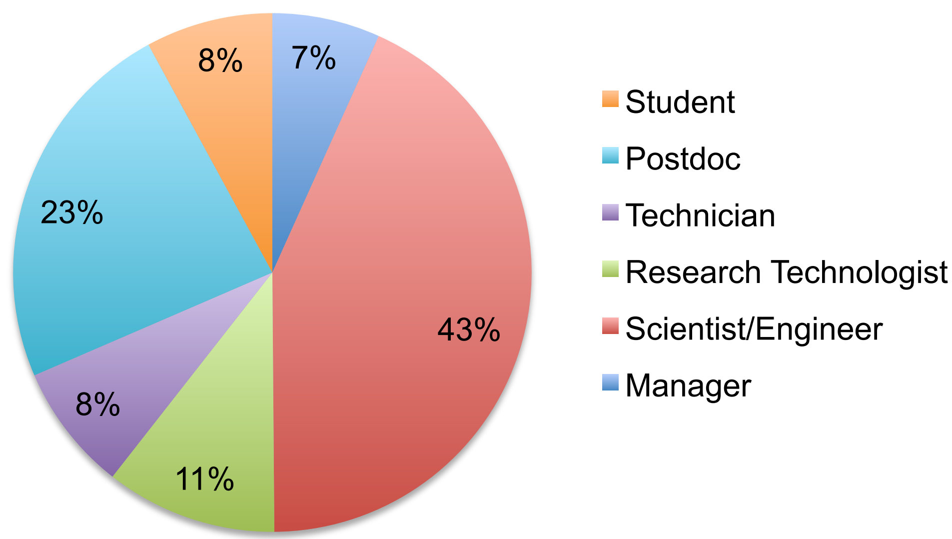
Materials have been important at LANL since the Manhattan Project!

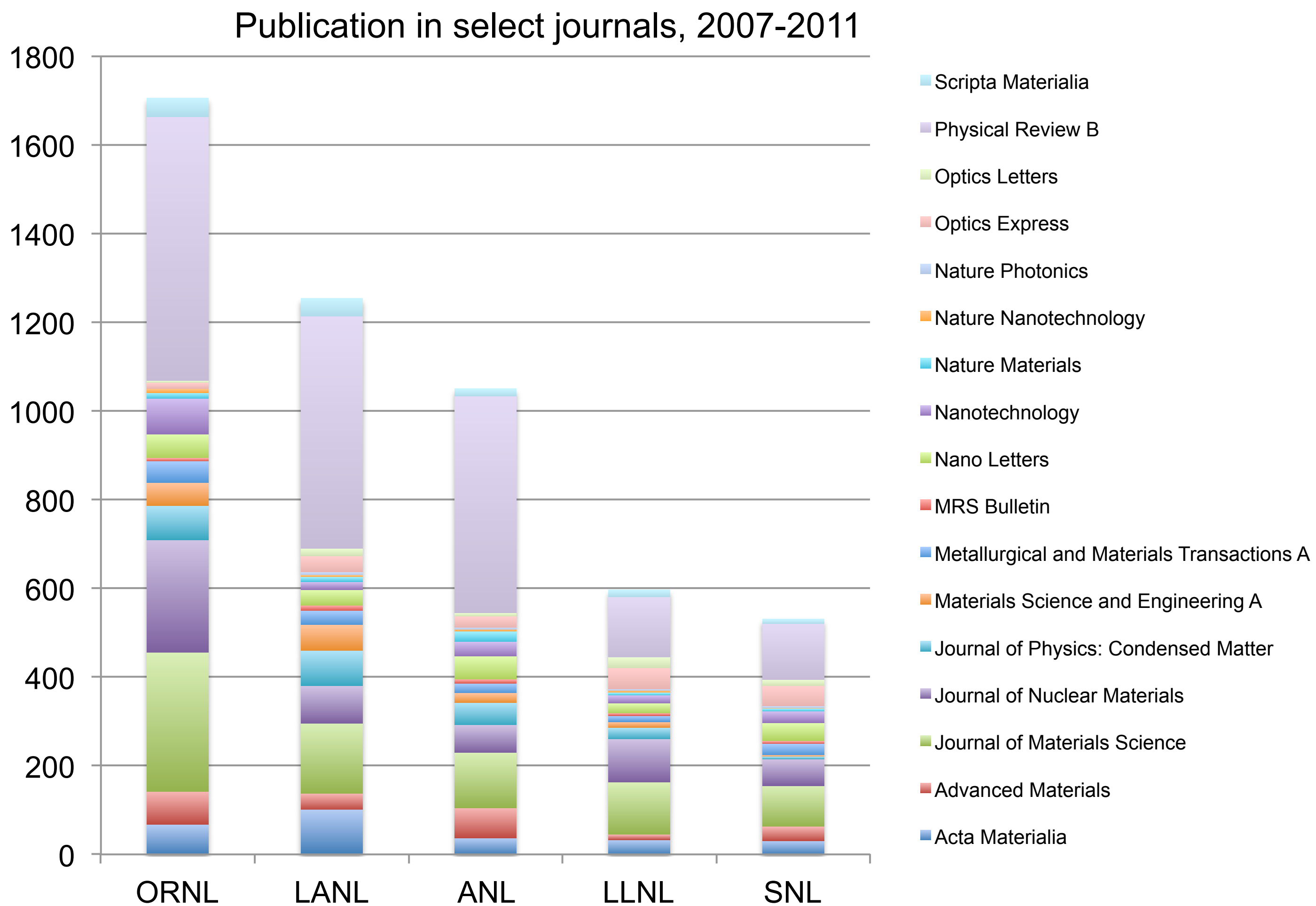


Materials R&D engages over ~830 personnel at LANL at a funding level of ~$260M

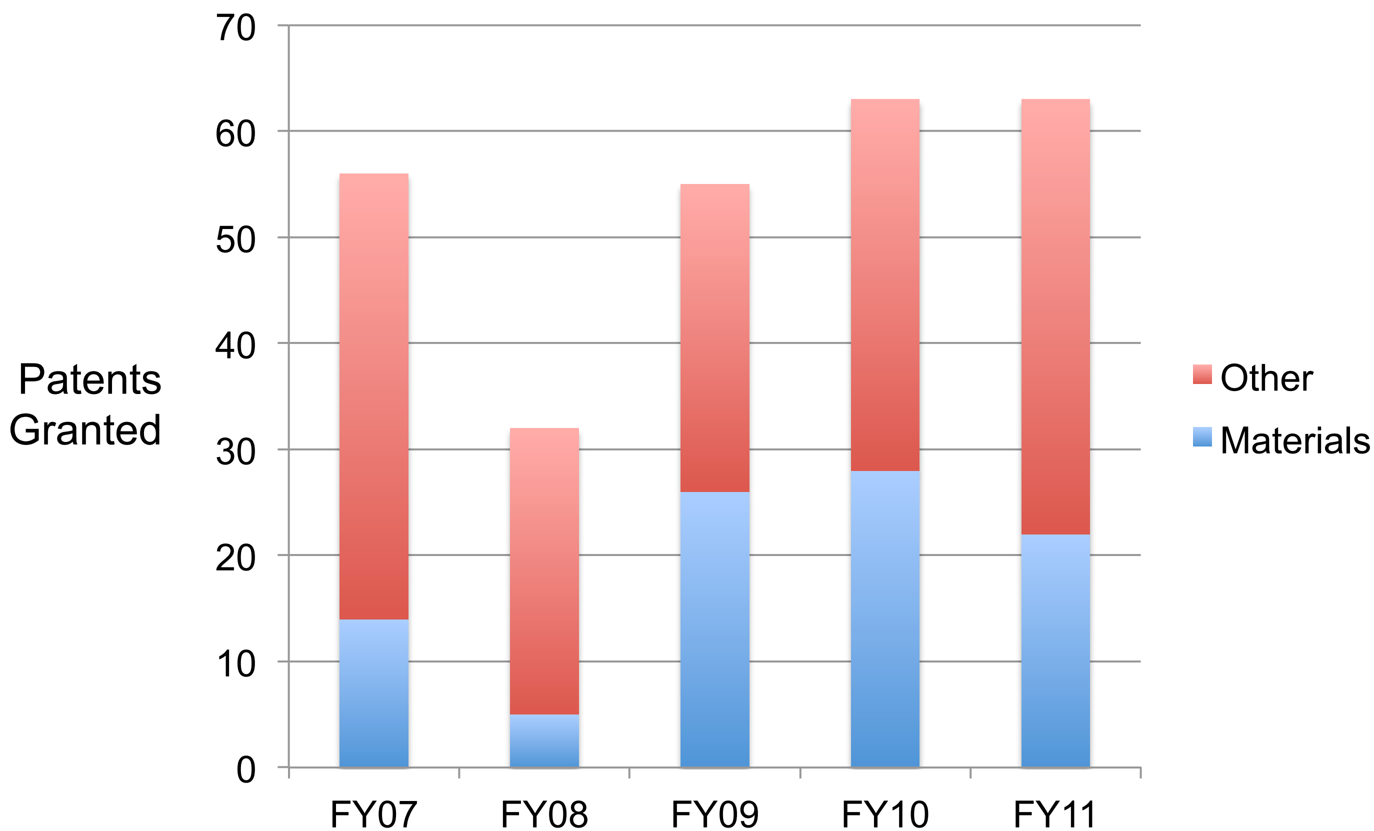




LANL is competitive with other national laboratories in materials publications

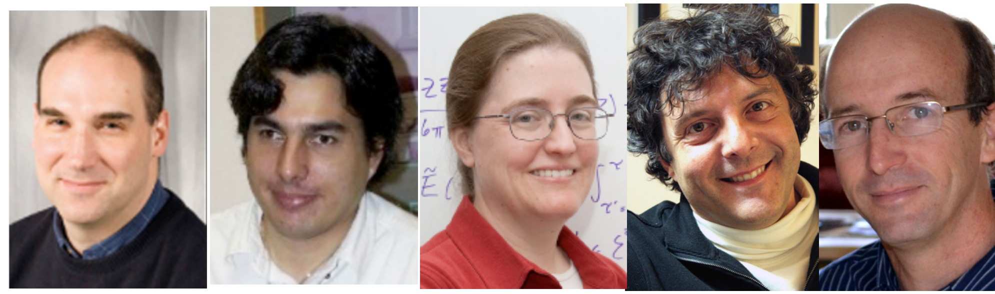


35% of patents granted to LANL over the past five years derive from materials research



LANL materials researchers continue to garner external recognition

Robert Field, Amit Misra, and Deniece Korzekwa: **ASM Fellows**



Timothy Germann, Charles Reichhardt, Cynthia Reichhardt, Bogdan Mihaila, and Marcelo Jaime: **APS Fellows**

Paul Burgardt: **American Welding Society Fellow**

Jeanne Robinson, Sasha Balatsky, Jacqueline Kiplinger, and Quanxi Jia: **AAAS Fellows**

John Carpenter and Nathan Mara: **TMS Young Leaders Professional Development Award**

Michael Nastasi: **MRS Fellow**

Dane Spearing: **American Ceramic Society Fellow**

David Chavez: **E.O. Lawrence Award**

LANL National User Facilities: a synergistic triad for materials research

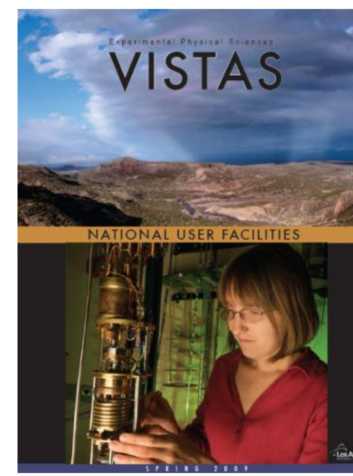
Nano-materials synthesis and characterization

Research with high magnetic fields

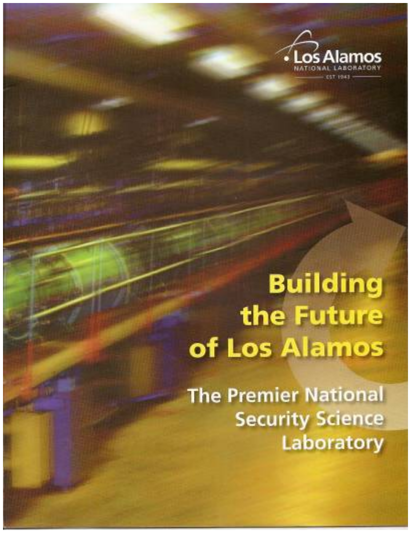
Materials @ LANL

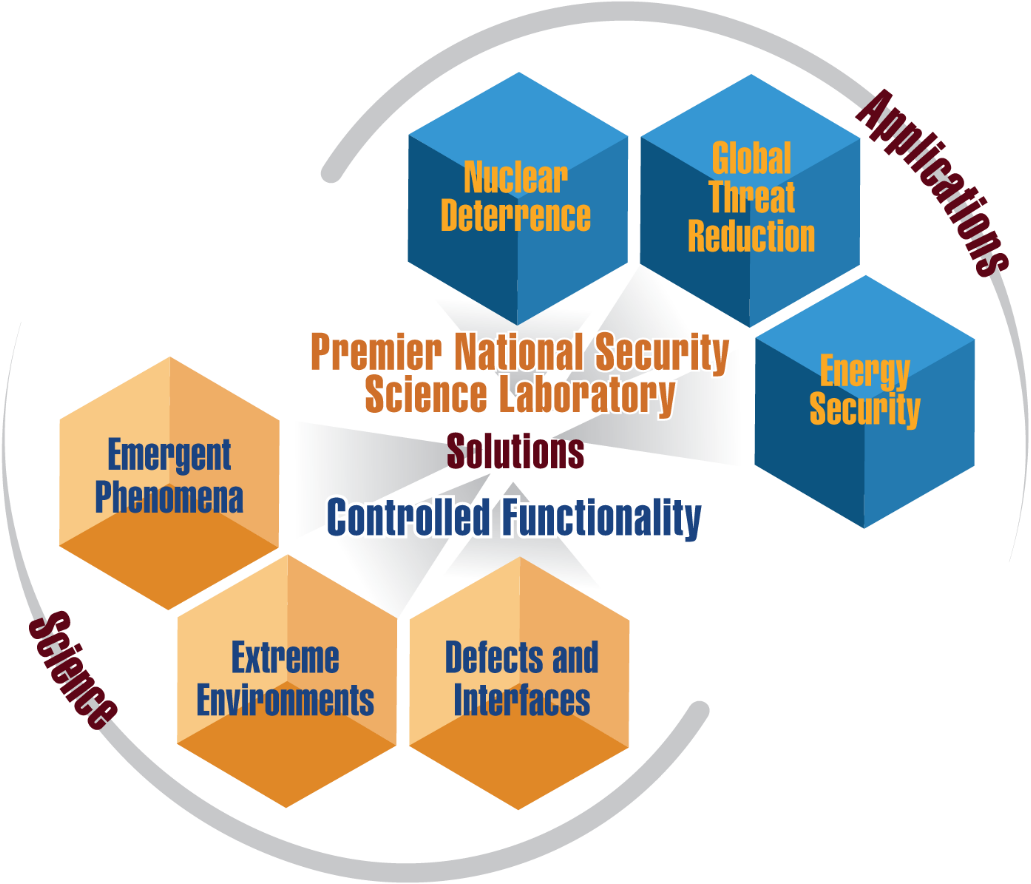
LUJAN CENTER
Los Alamos Neutron Science Center
Los Alamos National Laboratory

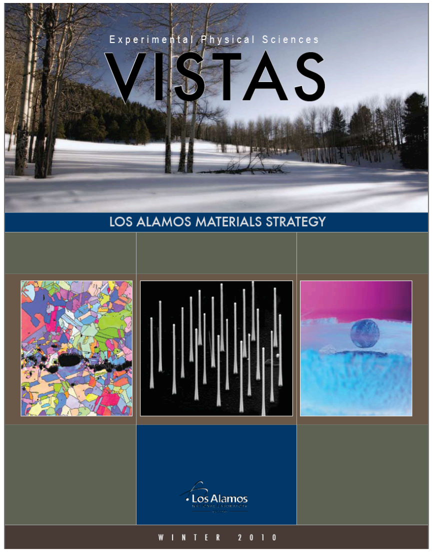
Neutron scattering



The Materials Strategy advances our vision to develop materials with 'controlled functionality' to provide solutions enabling LANL's missions

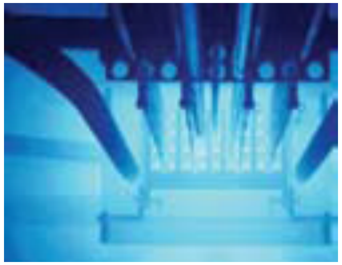






LANL Materials will be differentiated through forefront science that cross-cuts three themes

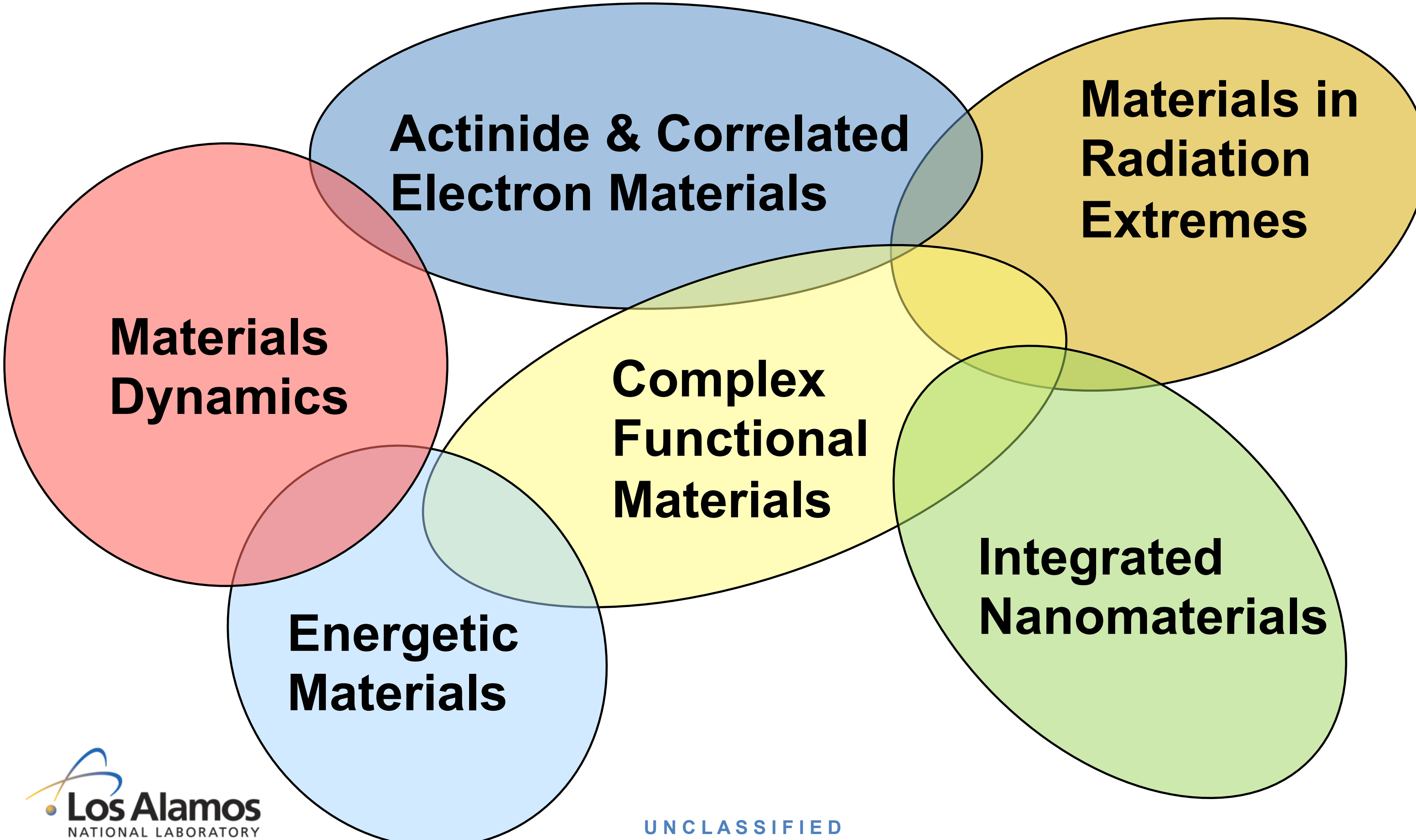
Defects and Interfaces – the mechanistic understanding and control of inhomogeneities, across all appropriate length and time scales, that govern materials functionality



Extreme Environments – the underlying principles enabling the understanding of the interactions of materials with extreme conditions in order to create 1) environmentally tolerant properties and 2) the ability to exploit extreme environments to tune materials functionality

Emergent Phenomena – the science required to discover and understand complex and collective forms of matter that exhibit novel properties and respond in new ways to environmental conditions, enabling the creation of materials with innate functionality

Six 'Areas of Leadership' span the Materials Pillar



Thrust areas further define the 'Areas of Leadership' for the Materials Pillar

- **Integrated Nanomaterials**
  - Reduced dimensionality materials for control of emergent functionality
  - Center for Nanophotonics
- **Complex Functional Materials**
  - Functional materials for energy conversion, storage and transmission
  - Materials inspired by living systems
  - Multifunctional adaptive materials
- **Materials in Radiation Extremes**
  - Advanced radiation & temperature tolerant structural materials
  - Advanced nuclear fuels & nuclear waste materials
- **Actinides and Correlated Electron Materials**
  - Understanding and controlling emergent electronic states
  - Actinide materials science center of excellence
  - Predicting and controlling plutonium aging and lifetime
- **Materials Dynamics**
  - Linking microstructure to macroscopic behavior under dynamic loading
  - Observation-to-control of dynamic processes
  - Next generation diagnostics and drivers
- **Energetic Materials**
  - Prediction and control of safety, initiation and performance of explosives

Materials Science and Technology (MST) Division

MST Division serves the nation by

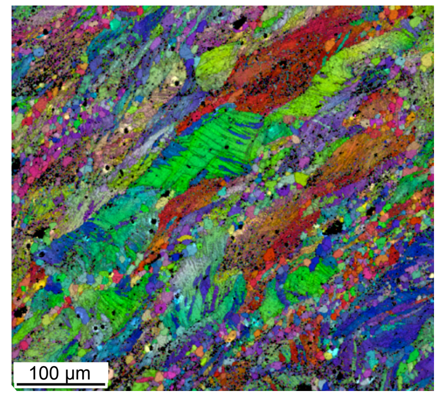
- **Delivering core materials science, technology, and hardware essential to ensuring and assessing weapons materials performance – expertise in actinides, beryllium, steels, intermetallic alloys, refractory metals, ceramics, and polymers;**
- **Integrating our understanding across materials synthesis, processing, properties, and performance to benefit programs from component manufacturing to fundamental materials science;**
- **Applying fundamental materials expertise to a range of national security needs including nuclear energy, nonproliferation, and global threat reduction;**
- **Developing advanced modeling, processing, coatings, corrosion compatibility, precision machining and assembly, and testing (static and dynamic) capabilities to create new knowledge, lay the foundations for new technologies, and deliver specialized hardware.**
- **Providing user-based materials characterization capabilities – including electron microscopy and ion beam characterization and implantation.**

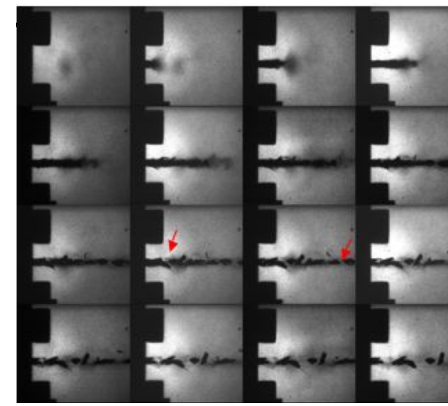
Key is the breadth and diversity of material scientists in MST Division that can bring knowledge and experience to solve a wide range of problems in national security

MST Division provides complete functionality expertise for multi-customer applications

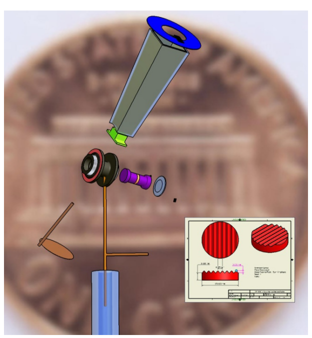
- **Materials Synthesis and Processing**

- **Microstructural and Property Characterization**

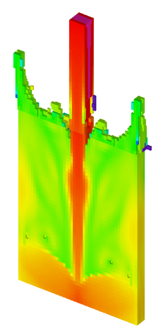


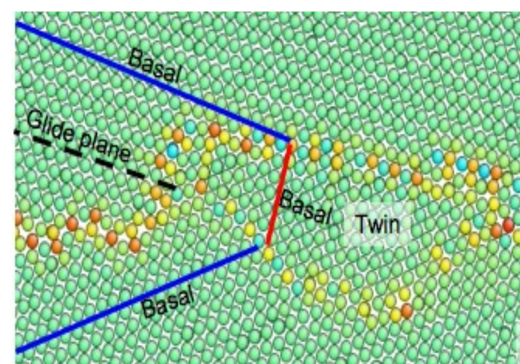


- **Component and Target Assembly**



- **Materials Modeling**





MST Core Competencies

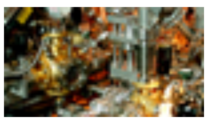
- Materials science, engineering, and technology of weapons materials
- Structural materials (Li to Pu): metals, ceramics and polymers
- Thin Films and Coatings
- Structure / property / processing fundamentals
- Materials modeling
- Weapons materials performance and aging assessments
- Materials manufacturing technology development
- Part fabrication
- Pit surveillance
- Corrosion / Materials Compatibility

http://www.lanl.gov/orgs/mst/

Metallurgy (MST-6)

<u>Alloy Design and Development</u> (arc-melting, directional solidification, melt spinning, zone refining, crystal growth; x-ray diffraction, x-ray fluorescence)

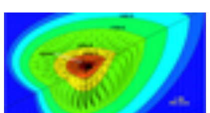
<u>Characterization</u> (optical and electron microscopy, metallographic preparation and etching)



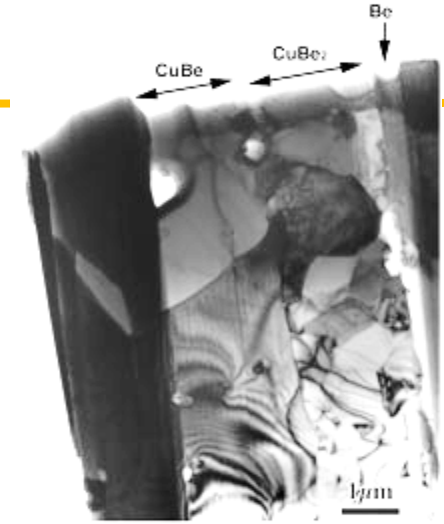
<u>Corrosion, Interfaces, and Electrochemistry</u> (electroplating, electropolishing, anodization, electroetching)

<u>Foundry/Machining</u> (casting, mold design, machining, forming machines, and furnace operations)

<u>Powder Metallurgy</u> (chemical processes, plasma spray, thermal spray)



<u>Welding and Joining</u> (gas tungsten arc welding, laser welding, electron beam welding, brazing)

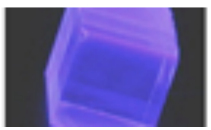


http://www.lanl.gov/orgs/mst/mst6/

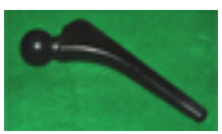
Polymers and Coatings (MST-7)

<u>Fundamental and Applied Polymer Research</u> (chemical synthesis, isotopic labeling, spectroscopy)

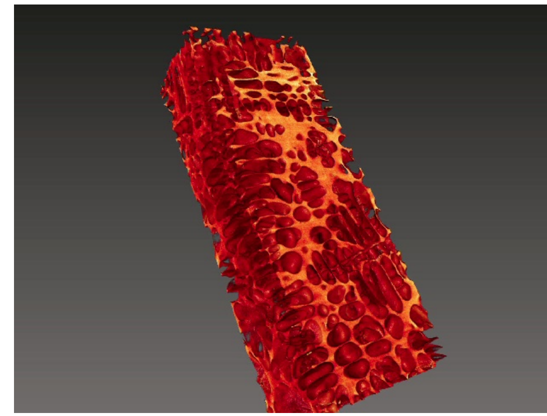
<u>Target Design and Fabrication</u> (machining, prototyping and exotic fabrication)

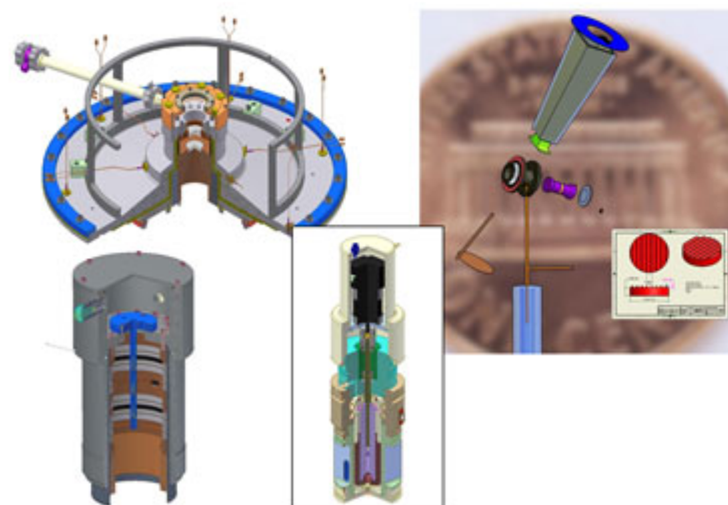


<u>Materials Characterization and Forensics</u> (materials synthesis, radiation response, optical and structural characterization)



<u>Surface Science and Coatings</u> (chemical vapor deposition, development of membrane materials, and characterization)





http://www.lanl.gov/orgs/mst/mst7/

Elucidating aging mechanisms is key to predicting service lifetime of polymers

- We employ a range of characterization techniques to determine aging or degradation mechanisms in polymers: NMR, FT-IR, GPC, Mossbauer, modulated DSC, TGA, BET, QCM, etc.
- Polymers of interest include polysiloxane foams, polymeric binders for high-explosives, elastomers.
- Example: Polysiloxane foams are degraded by tin catalyst residues used to synthesize these materials. These residues become catalytic inactive after about 20 years.

Solid-state NMR

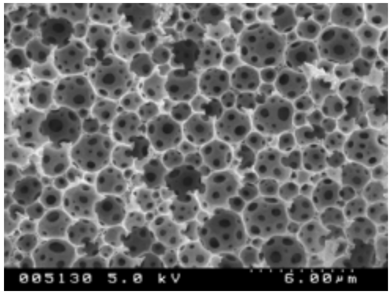
Modulated DSC

Dynamic Mechanical Analysis

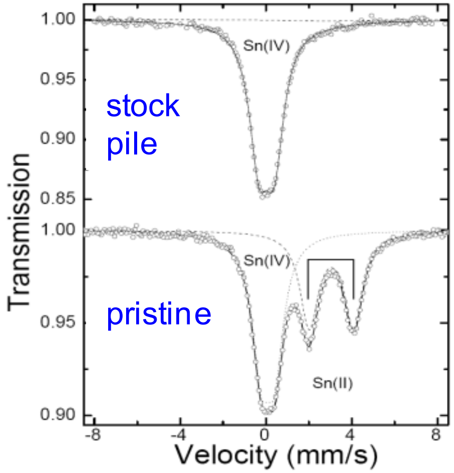
Gel Permeation Chromatography

Quartz Crystal Microbalance

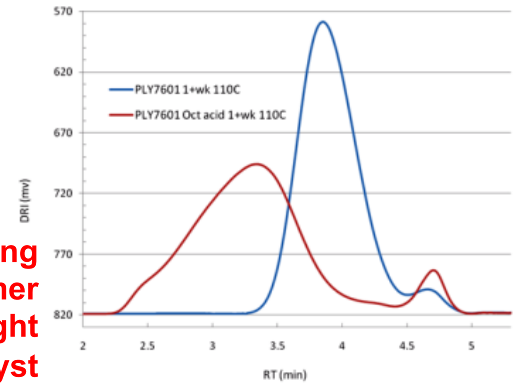
BET



Polysiloxane foam showing open cell structure



^{119}Sn Mössbauer data showing degradation of tin residues



GPC showing change in polymer molecular weight due to catalyst

Labouriau, MST-7

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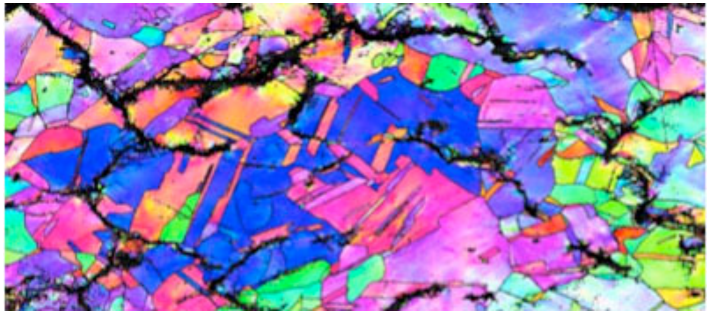
Materials Science in Radiation and Dynamics Extremes (MST-8)

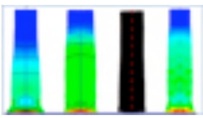
<u>Characterization and Modeling of Mechanical Properties</u> (modeling and simulations)

<u>Crystal Growth and Material Preparation</u> (synthesis of alloys/ceramics, characterization, single crystal growth)

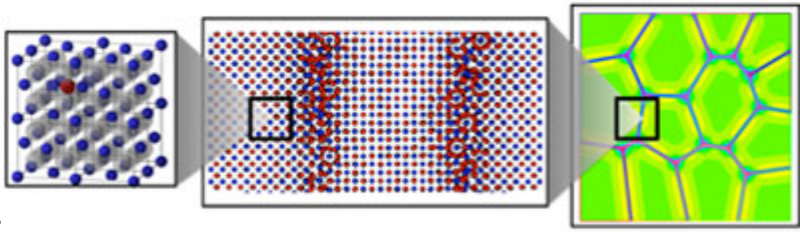


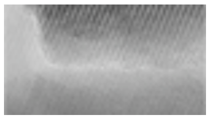
<u>Dynamic Materials Properties</u> (gas gun, Taylor anvil facility, Hopkinson pressure bars, mechanical test frames, characterization)

<u>Ion Beam Laboratory and Scanning Probe Microscopy</u> (ion beam analysis, tandem ion accelerator, ion implanter)



<u>Materials Modeling</u> (modeling and simulations)

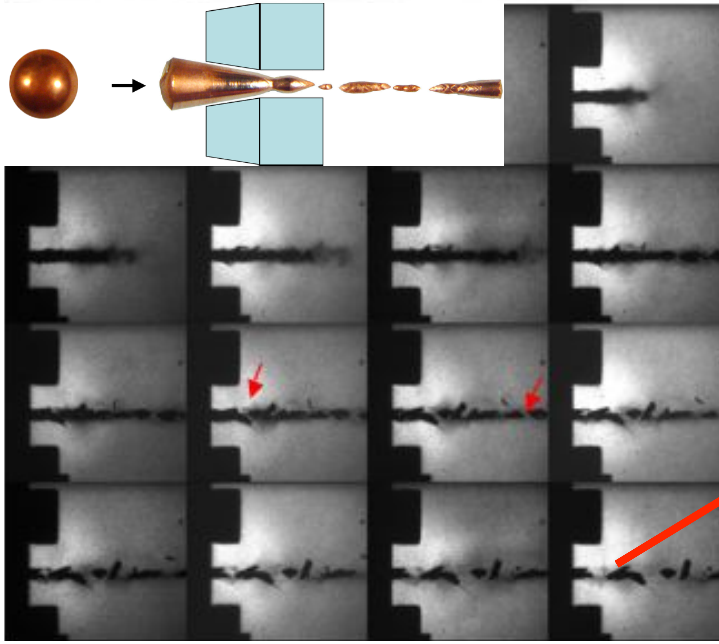


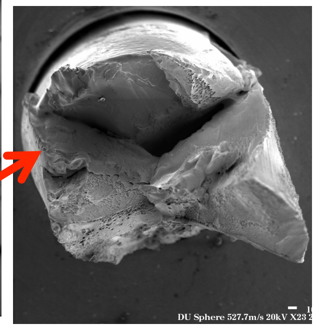


<u>Science of Defects in Materials</u> (synthesis and fabrication of oxide ceramics, ion beam irradiatior quantification of irradiation effects, characterizatic

http://www.lanl.gov/orgs/mst/mst8/

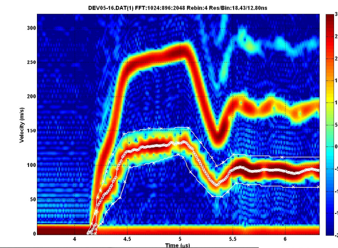
Dynamic tensile extrusion and incipient spallation experiments are informing predictive model development for Depleted Uranium.

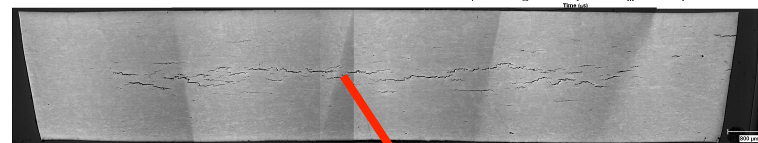


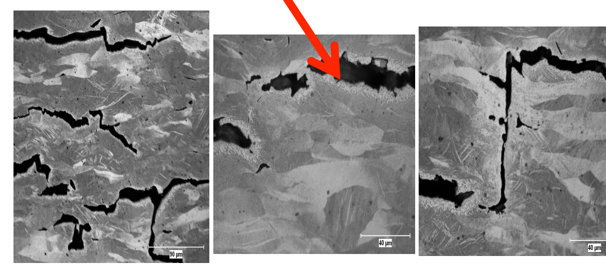


Dynamic Tensile Extrusion of DU

PDV velocity profile of incipient spall





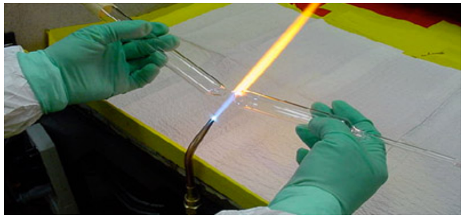


- Unlike similar experiments on Cu and Ta, DU breaks up into greater than 5 pieces and yet breaks appears to be shear dominated during dynamic extrusion.
- Incipiently spalled DU shows tensile cracking and severe plastic shearing often associated with inclusions and no evidence of microvoid formation and coalescence

Predictive modeling of dynamic damage evolution in DU requires complex shear processes to be described in next generation coupled strength / damage models under development.

Gray, MST-8

Nuclear Materials Science (MST-16)



Our mission is to provide

- **Multidisciplinary expertise in actinide materials science using a comprehensive suite of destructive and nondestructive analytical techniques within a category I nuclear facility; and**
- **Characterization of new and aged pit construction materials, the development of technologies for advanced actinide materials analysis, and the performance of actinide materials science investigations.**

Nuclear Materials Science Teams:

Dynamic Testing

Materials Properties

Metallography and Microscopy

Surface Science

http://www.lanl.gov/orgs/mst/mst16/

Materials Physics and Applications (MPA) Division: Mission / Research Areas

Mission:

Materials Physics & Applications Division will enable the development of new technologies that solve pressing National energy and security challenges by

- exploring and exploiting materials and their properties,
- developing practical applications of materials, and
- providing world-class user facilities

to enable the development of new technologies that solve pressing National energy and security challenges

MPA research areas include:

- Condensed Matter Physics
- Actinide Science
- Nanoscience integration
- Electrochemical Materials
- Applied Superconductivity
- Sensor R&D
- Materials Chemistry
- Magnet Science and Technology
- Materials Integration/Device development
- Biomaterials/Soft Matter
- Advanced Spectroscopies
- Materials Integration & Processing

http://www.lanl.gov/orgs/mpa/cmms/

Condensed Matter & Magnet Science

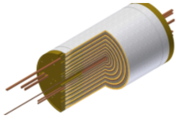
Our mission is to provide

- **Extreme magnetic fields at the Pulsed-Field Facility in support of the National High Magnetic Field Laboratory's User Program**
- **Expertise in strongly correlated electronic systems in support of fundamental science and LANL energy security missions. Emphasis is on discovering new physics through new materials**
- **Expertise in actinide science through a combination of crystal growth, spectroscopy, characterization, and extreme sample environments**

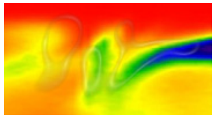
Areas of Specialization:

NHMFL User Program

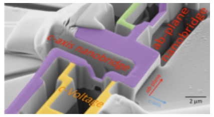
Strongly Correlated Electronic Systems



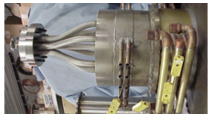
Magnet Engineering



Low Energy Spectroscopy



High-Field Science



Thermal Physics & Energy Applications

Los Alamos NATIONAL LABORATORY EST.1943

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NNSA

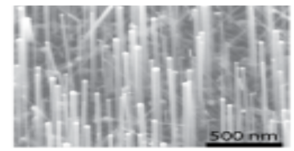
http://cint.lanl.gov/

The Center for Integrated Nanotechnologies (CINT)

Our mission is to provide

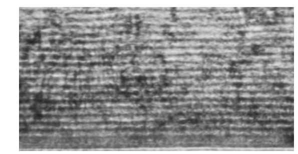
- **An internationally recognized Office of Science Nanoscale Science Research Center User Facility serving a broad research community and developing an internal science program that advances the state of nanoscience R&D**
- **A successful, high-visibility Energy Frontier Research Center, the Center for Materials under Irradiation and Mechanical Extremes, to establish the principles underlying materials performance under extreme conditions**
- **State-of-the-art capabilities in ultrafast science through our Laboratory for Ultrafast Materials and Optical Science for characterization and exploitation of functional and emergent materials**
- **Our expertise in synthesis and characterization of novel bulk and nanoscale materials in support of Lab missions in Nuclear Deterent, Global Security, and Energy Security**

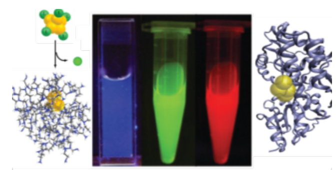
Areas of Specialization:



Nanostructured Functional Materials

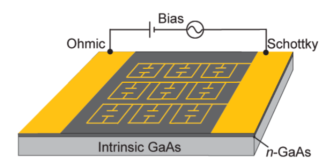
Nanoscale Structural Materials

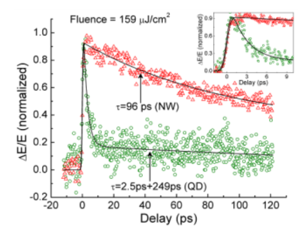




Soft & Biological Nanomaterials and Composites

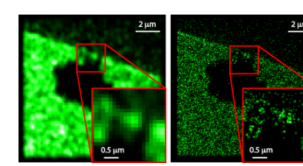
Metamaterials



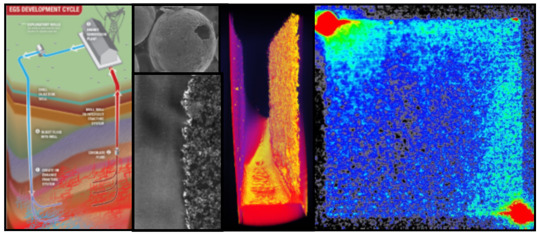


Ultrafast Science

Single Molecule/Nanoparticle Microspectroscopies and Scan Probe Systems



http://www.lanl.gov/orgs/mpa/mpa11/



Sensors & Electrochemical Devices

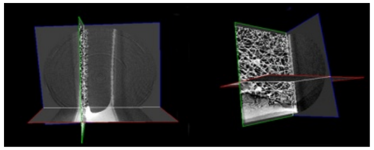
Our mission is to

Apply fundamental knowledge of materials science and electrochemistry to National Security challenges through

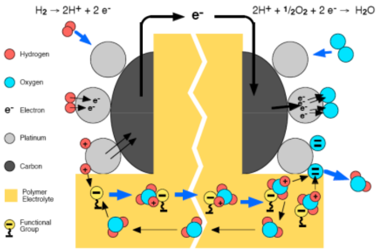
- **basic and applied research on electronic and ionic conducting materials, and**
- **development of novel materials characterization approaches.**
- **focus on alternative energy systems and sensors**
- **proof-of-concept device development**

Our research forms a basis for development in device technology and practical application of materials.

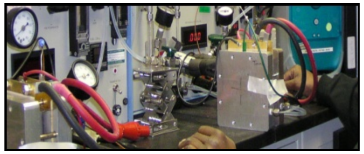
Areas of Specialization:



Materials Chemistry



Electrochemistry

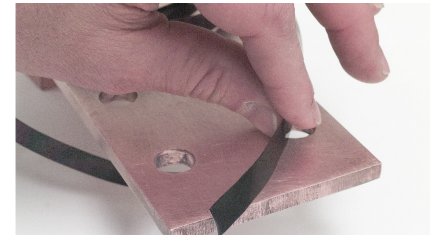


Fuel Cells

Acoustics & Sensors Technology

http://www.lanl.gov/orgs/mpa/stc/

Superconductivity Technology Center

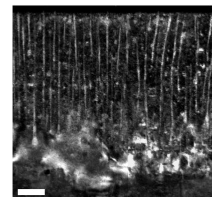


Our mission is to provide

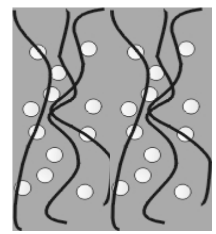
- **Energy efficient technologies in collaboration with American industry and universities and in support of the LANL energy security mission.**
- **Research and development of advanced conductor materials, including high temperature superconductor and carbon nanotube composites**
- **Development of magnet and power applications using advanced conductor technologies**

Areas of Specialization:

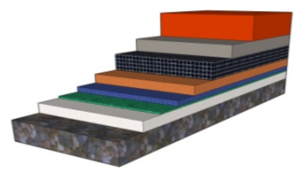
STC



Materials Development



Vortex Physics



Coated Conductor

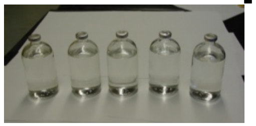
Power Applications

Materials Chemistry

Our mission is to provide innovative and creative chemical synthesis solutions to solve materials problems across the mission.

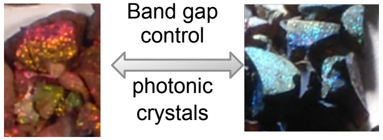
- **Global Threat Reduction**
  - Extraction and separation strategies using ionic liquids
  - Chemical amplification of signals
  - New composite phosphors for radiation detection
  - Novel signatures based on chemical reactivity
- **Nuclear Deterrence**
  - Material development for stewardship and safety
  - Process aware material performance
  - Plutonium science and f electron interactions
- **Energy Security**
  - Membranes for CO_2 sequestration and separation
  - Hydrogen storage materials
  - New electrodes for energy storage
  - Membranes for alkaline fuel cells

Thrust Areas:

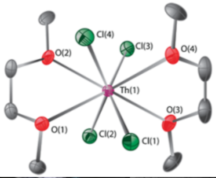


Bulk high purity ionic liquids

Molecular synthesis



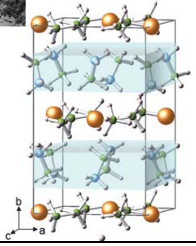
Composite materials



Actinide chemistry

Material development

Membrane materials



Energy storage

National High Magnetic Field Laboratory

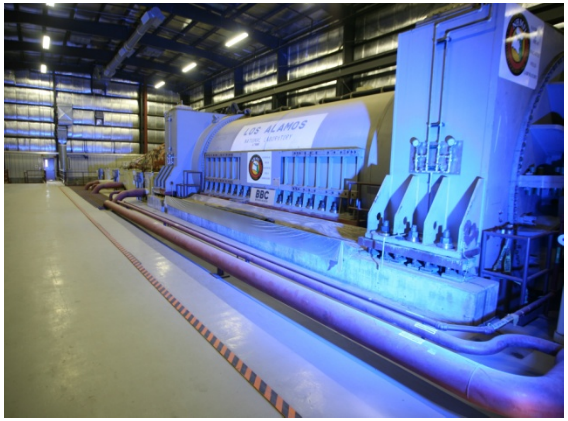
Our mission:

- Provide qualified users with *Extreme High Magnetic Field* research environment
- Drive Extreme High Magnetic Field generation technology

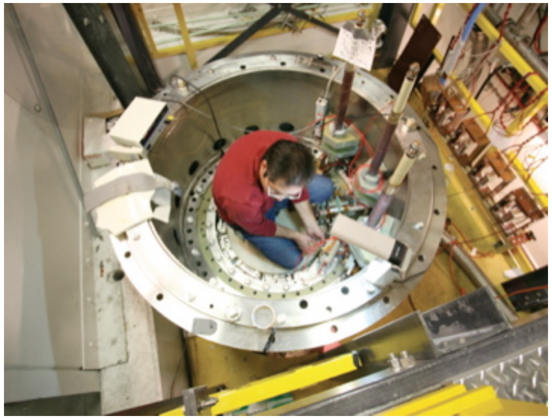
Statistics:

- 150 users per year from all corners of the globe
- $6M year NSF funded program
- 11 Scientific staff provide expert user support
- 50-60 peer reviewed publications per year

1.43 GigaWatt Generator



Unique Magnet Capabilities

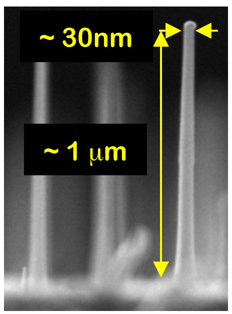


CINT's focus is on nanoscale integration—the key to exploiting nanomaterial functionality

The science of nanomaterials integration:

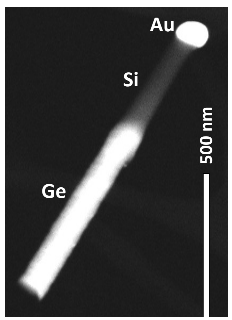
Combining diverse nanomaterials together across length scales and into nanosystems to achieve novel properties and performance.

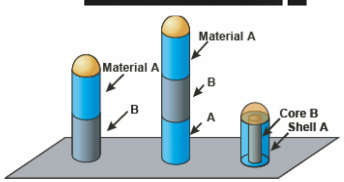
Synthesis



Ge NWs on Si(111)

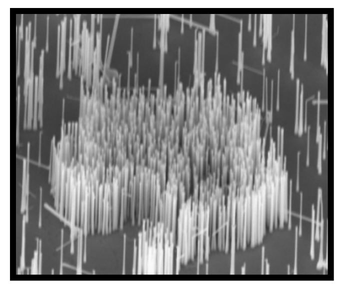
Heterostructure





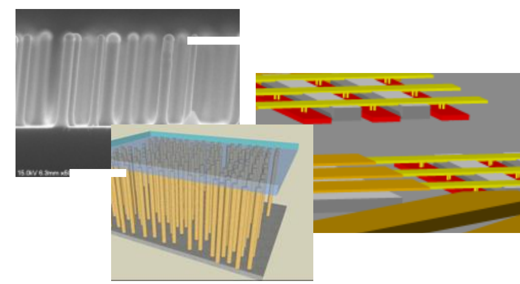
Axial & core/shell heterostructures,

Assembly



Ge nanowire nanobiotemplated array

Nanosystems



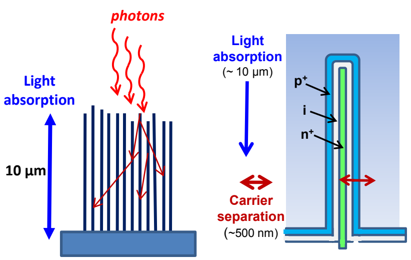
Vertical crossbar arrays

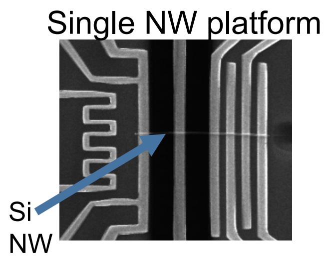
Length scale

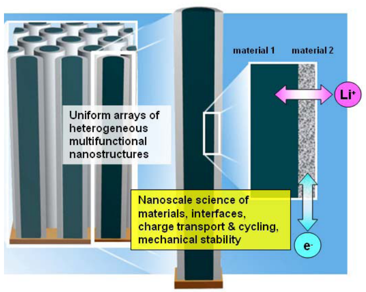
Nanoscale → **Micro/Macroscale**

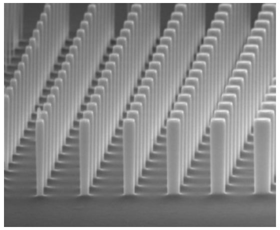
Semiconductor Nanowires for Energy Applications

- **Explicit development of nanowire energy applications: Tom Picraux**
  - **Photovoltaics**
  - **Thermoelectrics**
  - **Li ion battery anodes**
  - **Solid state lighting**

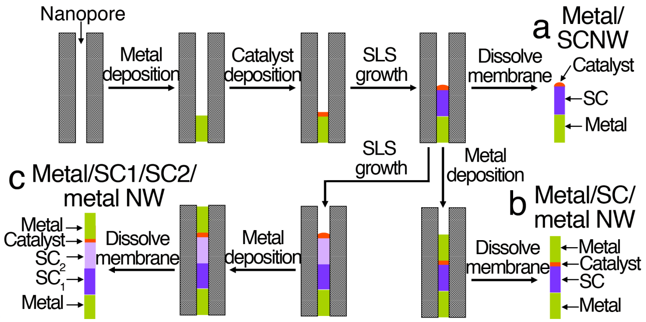


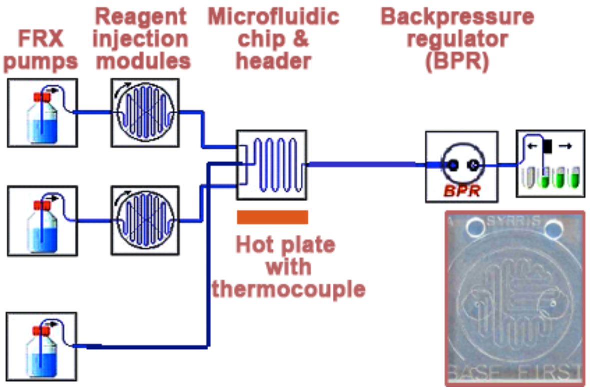






- **New solution-based fabrication strategies: Jen Hollingsworth**
  - ***In situ* metal-semiconductor contacts**
  - **Microfluidics-based solution-liquid-solid growth**





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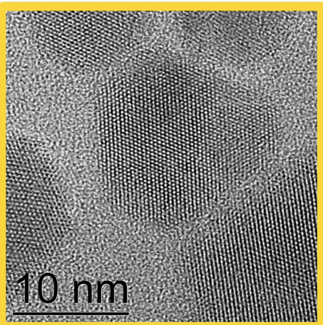
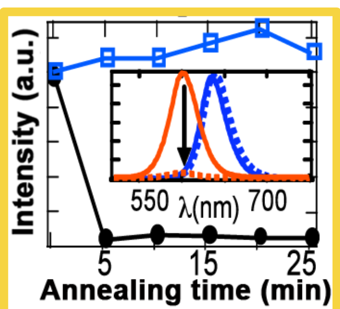
Energy Conversion: Giant Quantum dots (BES Core Program)

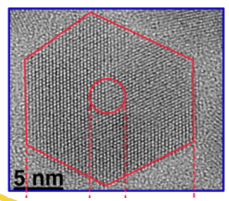
Epitaxial-quality" QDs grown in a flask



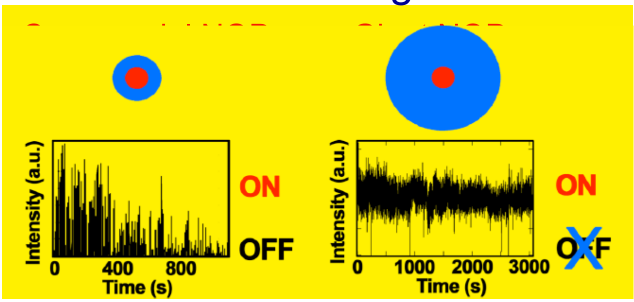
Robust to chemical & thermal treatments



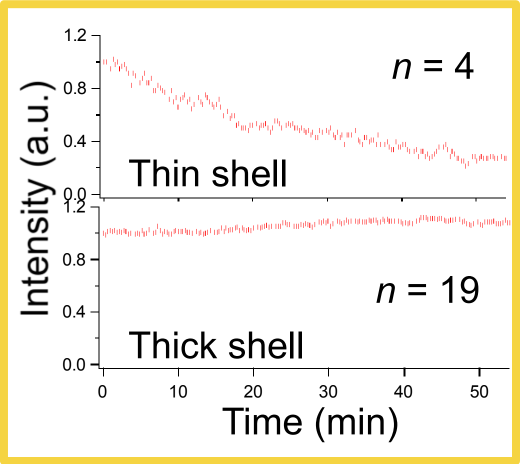
Novel physical & electronic nanostructure affords new functional class of QD for device (LED, single-photon, lasing) and tracking applications



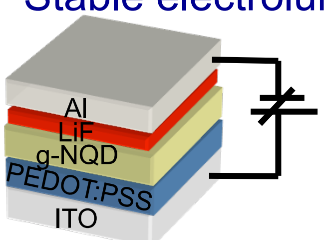
Non-blinking

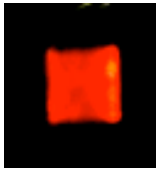


Non-photobleaching



Stable electroluminescence





Chen et al. *J. Am. Chem. Soc.* (2008) 5026

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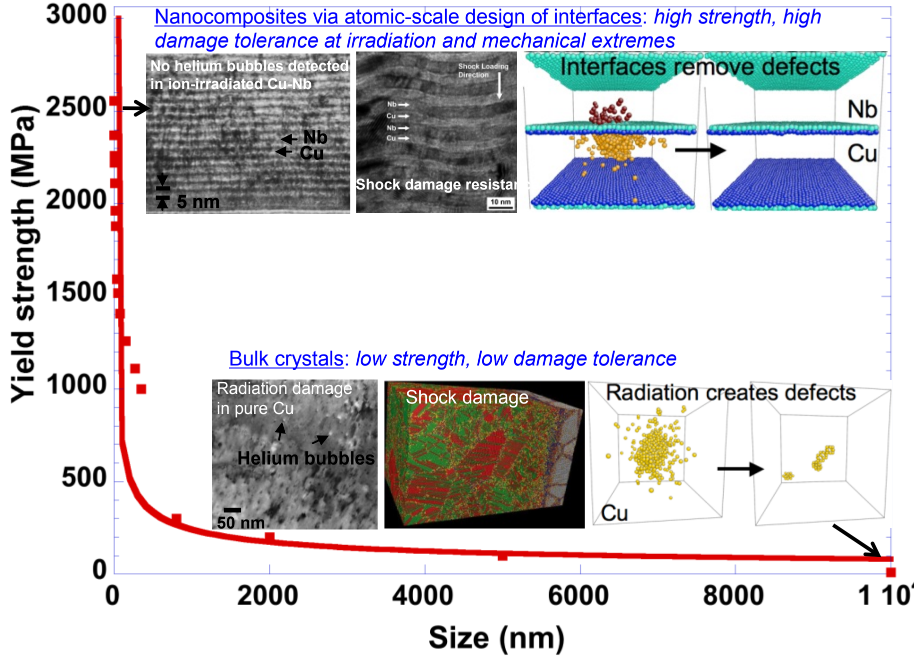
Center for Materials at Irradiation and Mechanical Extremes

BES Energy Frontier Research Center

The purpose of this EFRC is to understand, at the atomic scale, the behavior of materials subjected to extreme radiation doses and mechanical stress in order to synthesize new materials that can tolerate such conditions.



The EFRC is developing a fundamental understanding of how atomic structure and energetics of interfaces contribute to defect and damage evolution in materials, and use this information to design nanostructured materials with tailored response at irradiation and mechanical extremes with potential applications in next generation of nuclear power reactors, transportation, energy and defense.

-http://cmime.lanl.gov

Fuel Cell Program

One of longest running non-weapons programs at LANL (since 1977)

- Based out of MPA-11, includes MPA, MST, T, C Divisions
- Yearly budget of \$7M - \$11M, ~ 45 researchers involved at LANL

Fuel Cells R&D Projects Focus on Cost and Durability

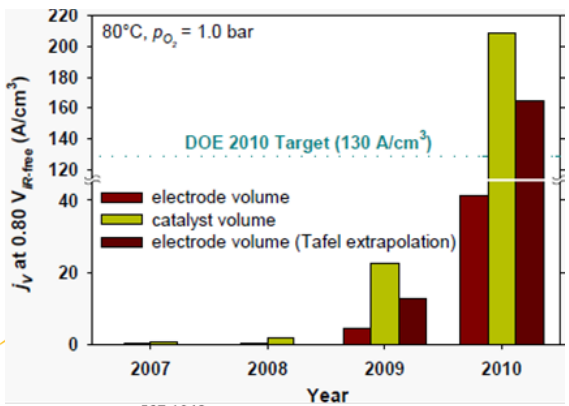
- Fuel cell durability
- Electrocatalysis
- Alternative membranes
- Impurity effects
- Water transport
- Portable power

Lengthy History of Partnering with Major Developers:

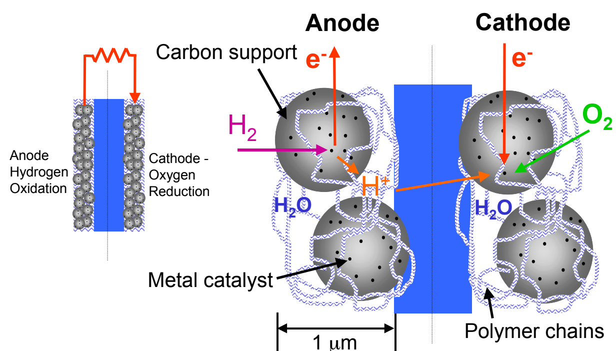
General Motors, Ford, 3M, Delphi Automotive, W.L. Gore, BASF, SGL Carbon GMBH, UTC, AFCC, Ballard Power Systems, Ceramatec Inc., IRD Fuel Cells, Nissan Motor Company, Hyundai Motors Company, other National Labs, Universities

~ 90% of LANL Fuel Cell Funding is awarded by DOE EERE competitive solicitations.
Future Issues: Declining EERE Fuel Cells Budget, Required Cost Share

Tremendous Progress in Non Precious Metal Catalysis



LANL Breakthrough Thin Film Electrode



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Fuel Cells for Transportation

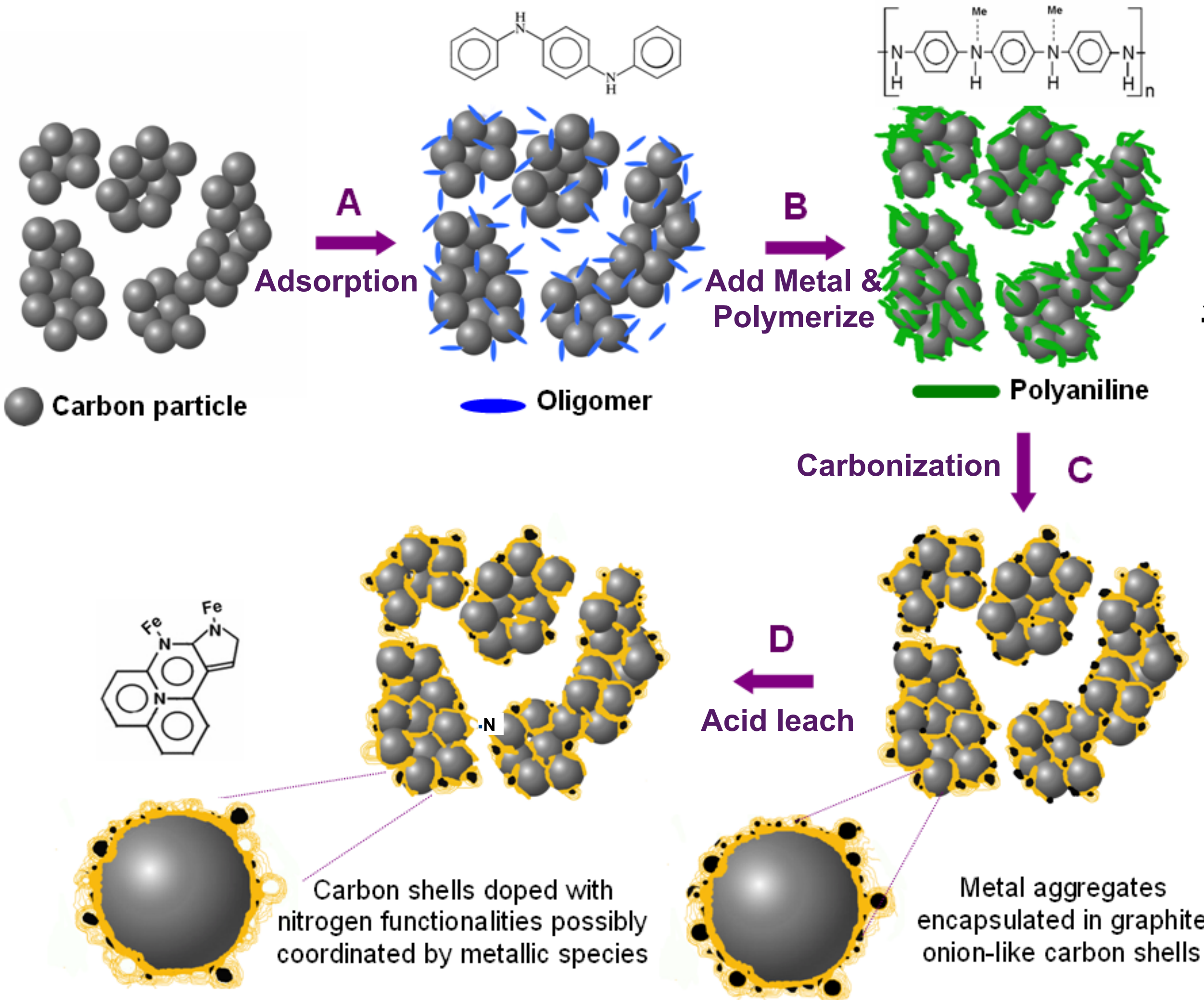
In the U.S., there are currently:

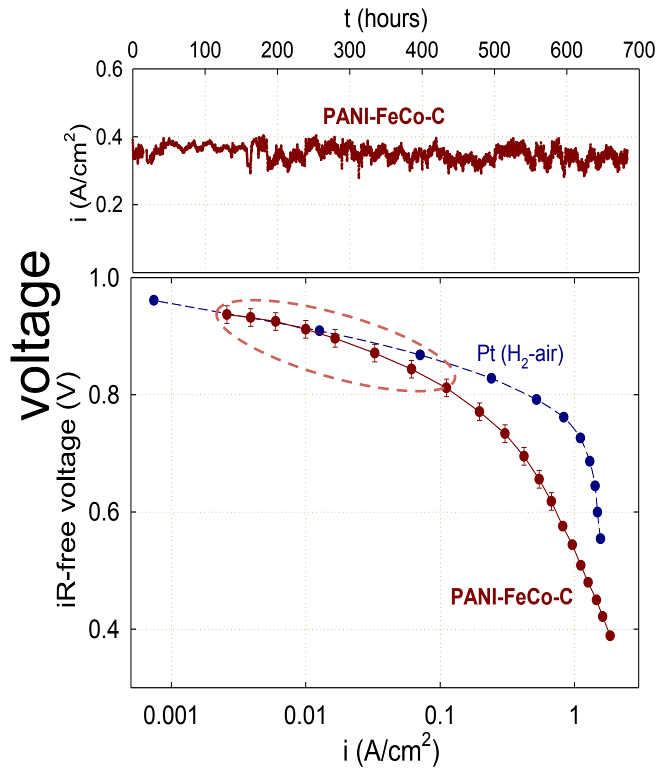
- ***> 150 fuel cell vehicles***
- ***~ 15 active fuel cell buses***
- ***> 50 fueling stations***

Sept. 2009: Auto manufacturers from around the world signed a letter of understanding supporting fuel cell vehicles in anticipation of widespread commercialization, beginning in 2015.

(US Patents #4,876,115, #5,211,984 and #5,234,777)
Used in virtually every PEM fuel cell today

Energy Conversion: First stable, high-performance non-precious metal fuel cell cathode

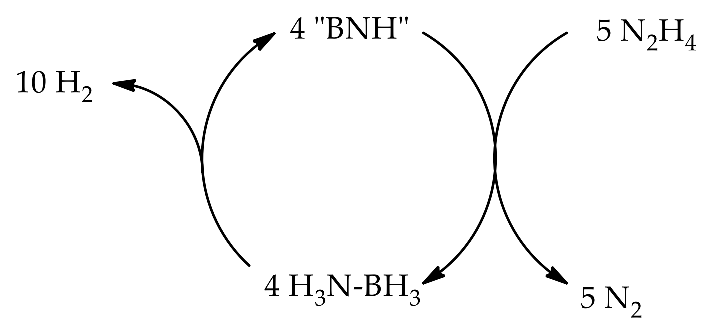




High-Performance Electrocatalysts for Oxygen Reduction Derived from Polyaniline, Iron, and Cobalt, G. Wu, K. L. More, C. M. Johnston, and P. Zelenay, *Science*, 332, 6028, 443-447 (2011)

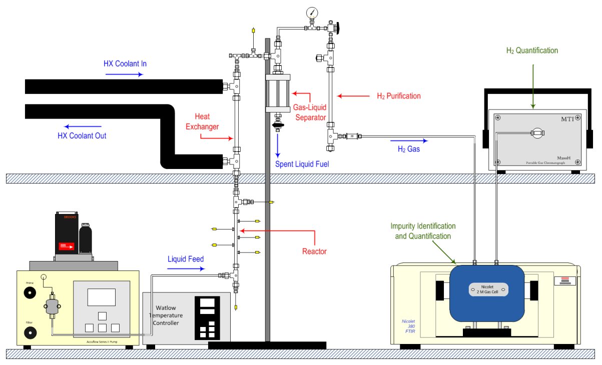
Chemical H_2 Storage Research at LANL

- **Center of Excellence in Chemical Hydrogen Storage**
  - New fluid phase formulations
  - Long term stability measurements
  - One pot efficient regeneration method
  - Future: increased H_2 capacity



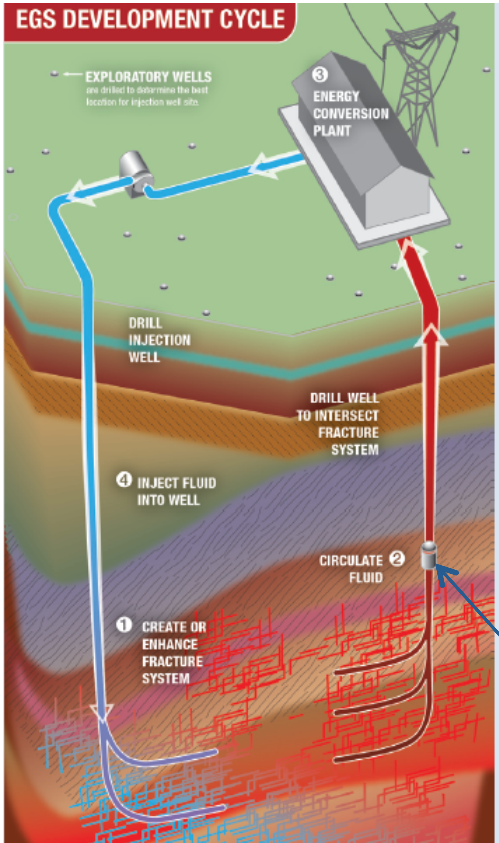
Science, March 18, 2011

- **Hydrogen Storage Engineering Center of Excellence**
  - Small-scale demo, novel fuel sensor design, impurity mitigation
  - Future: startup/shut down and heat management must be addressed



High Temperature Downhole Tools: Multipurpose Acoustics Sensor

U.S. DOE Energy Efficiency and Renewable Energy (EERE) project
American Recovery and Reinvestment Act (ARRA)



LANL sensor

Development of a multipurpose (simultaneous multiple physical parameter determination) acoustic sensor for downhole fluid monitoring in Enhanced Geothermal Systems (EGS) reservoirs at high pressure-high temperatures conditions.

In-situ single sensor for simultaneous determination of:

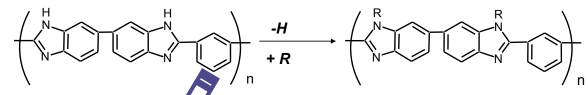
- **Borehole temperature**
- **Borehole pressure**
- **Fluid properties:**
  - **- sound speed**
  - **- sound attenuation**
  - **- density**
  - **- viscosity**
- **Fluid composition**
- **Fluid flow**

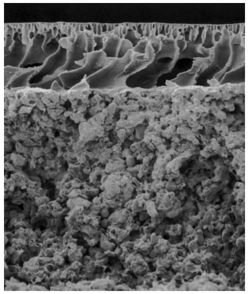
Membrane Materials for Energy Applications

Technically and Economically Viable Separations Technology Development

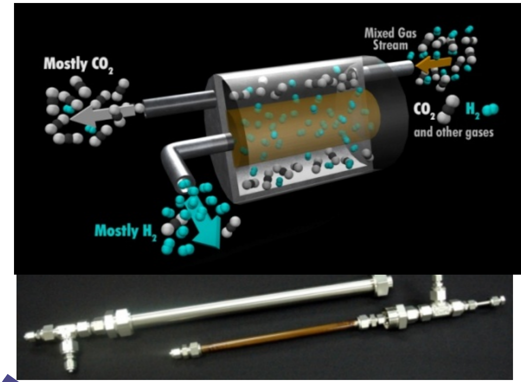
- **Enabling technologies for more efficient and cleaner energy, chemicals, fuels, bio-chemicals, and bio-fuels production**
- **Rational design, synthesis, development, and demonstration of selective barrier materials**
- **Membrane and module development**
- **Long-term membrane performance prediction and optimization**
- **Systems integration & optimization**

Rational Materials Design



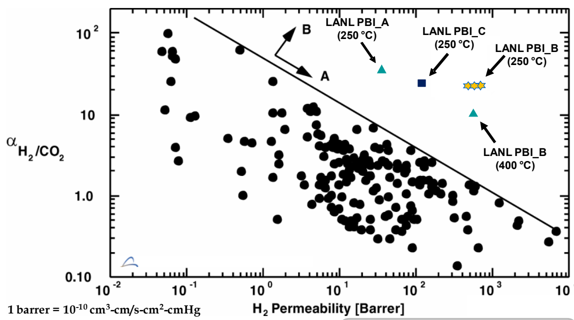


Morphology Optimization

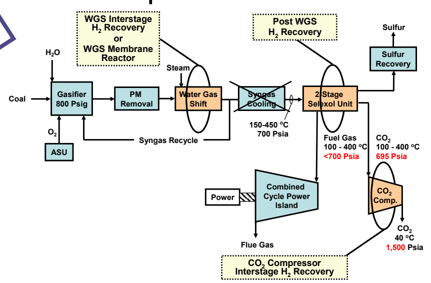


Membrane and Module Design, Evaluation, & Scale-Up

Demonstrate improvements over the state-of-the-art while operating at industrially attractive conditions



Systems Integration and Optimization

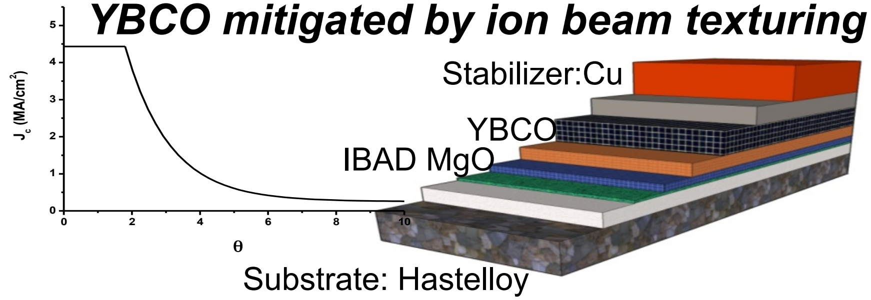


High Temperature Superconductors

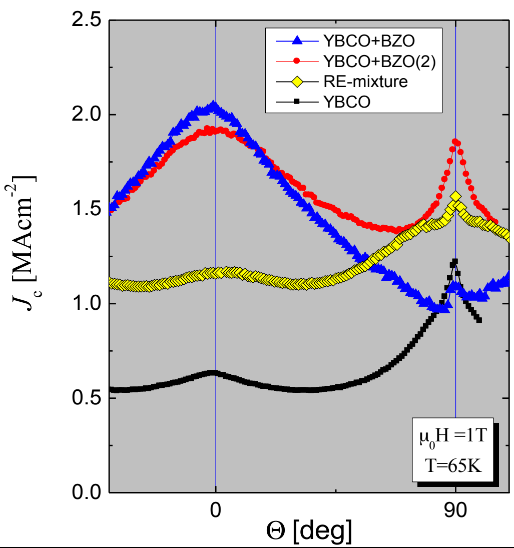
Motivation

- no electrical resistance (cooled with liq N2)
- 250x the current density of copper
- more powerful, efficient, smaller, lighter
- increased energy infrastructure security

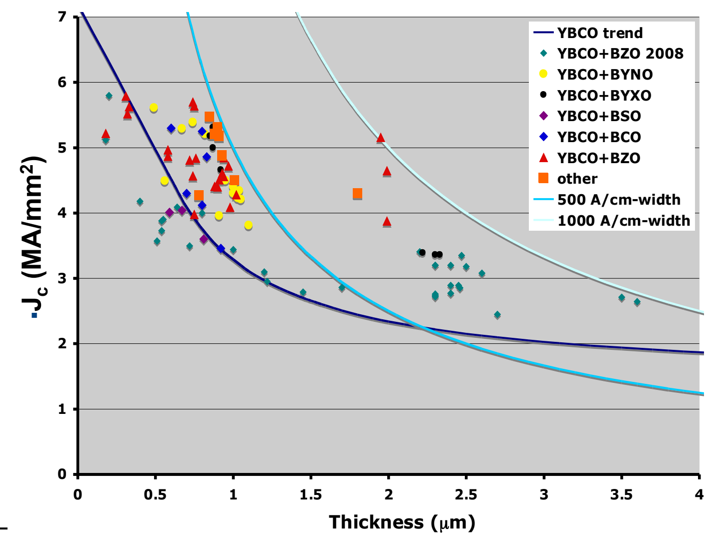
Current decrease across GBs in YBCO mitigated by ion beam texturing



Anisotropy in current density controlled by vortex pinning defects



Current decrease with thickness mitigated by microstructure control



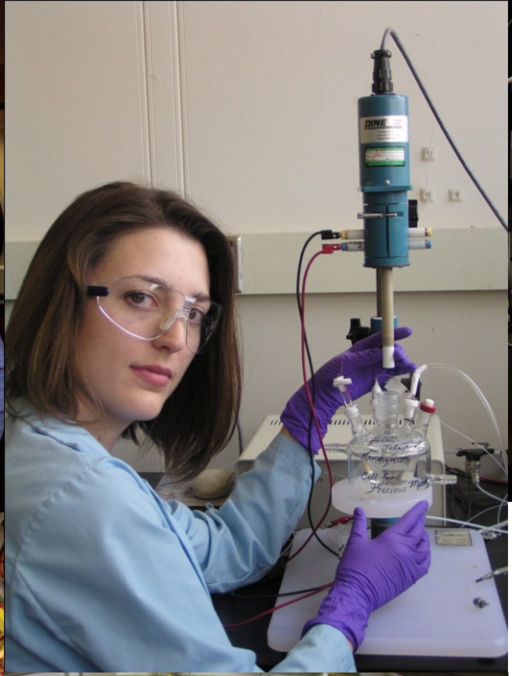
From 2005- 2010 in-field Ic at LANL was increased by 10x

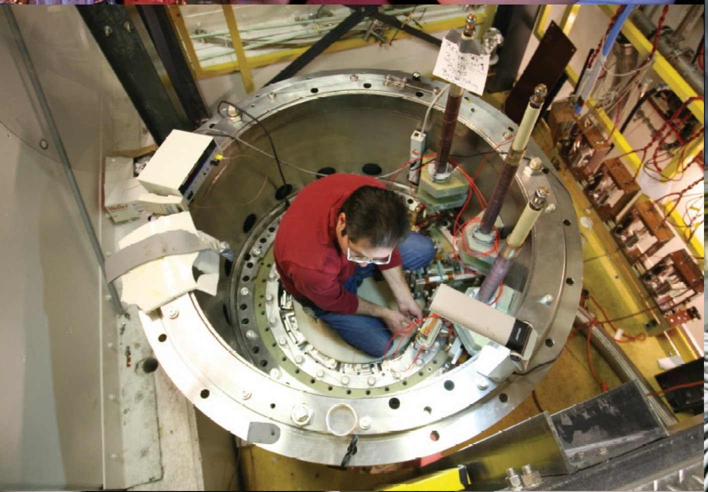
Industrial & utility collaborations have been critical to Materials S&T and programs

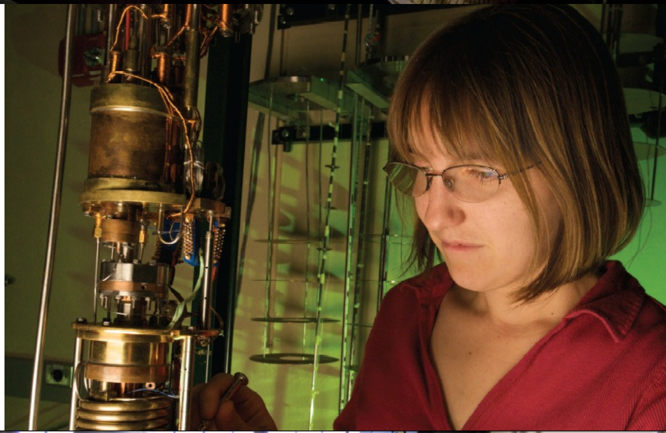
3M
DUPONT
The miracles of science
AEP AMERICAN ELECTRIC POWER
GENERAL DYNAMICS
Strength On Your Side
SOUTHERN CALIFORNIA EDISON
An EDISON INTERNATIONAL Company
EPRI ELECTRIC POWER RESEARCH INSTITUTE
LIPA
Long Island Power Authority
PNM
LOCKHEED MARTIN
We never forget who we're working for
ABB
Power and productivity for a better world
BOEING
GE
hp
CeraCon
PIRELLI
ERIEZ
PRAXAIR
BOC
AIR PRODUCTS
GENERAL ATOMICS
AND AFFILIATED COMPANIES
Astronautics Corporation of America
Hyper Tech Research, Inc.

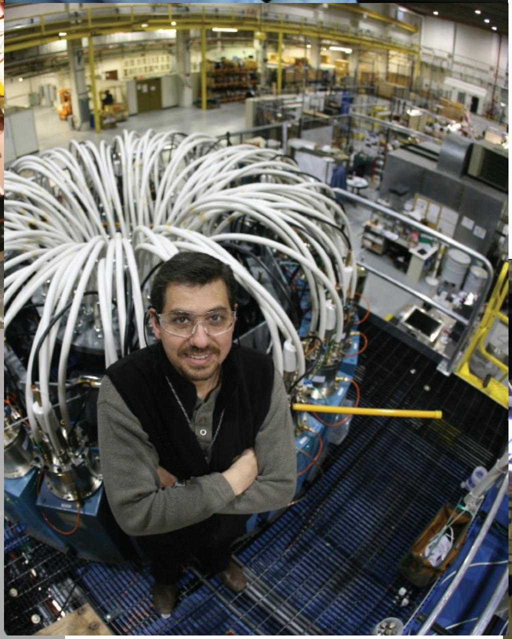
SuperPower Inc
STI
SUPERCONDUCTOR TECHNOLOGIES INC.
American Superconductor
SCI Engineered Materials, Inc.
metox
Making The Promise of Superconductivity A Reality
ZENERGY POWER
OXFORD INSTRUMENTS
Southwire
WE DELIVER POWER

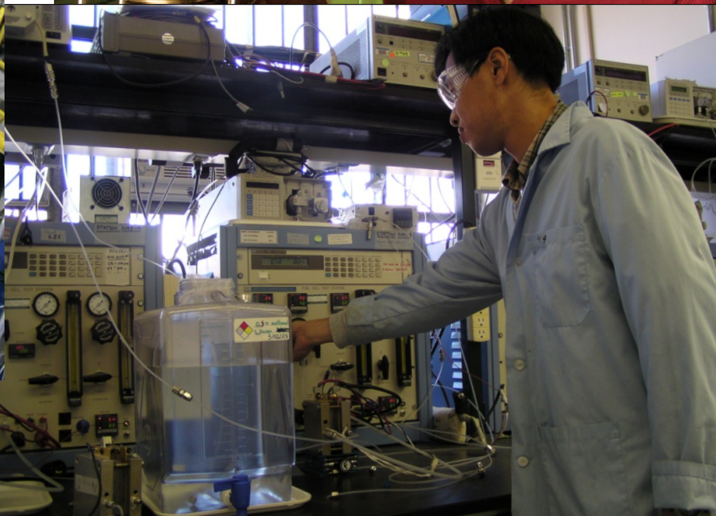
Chevron
Human Energy











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nt of Energy's NNSA